

# Dephasing in Metals by Two-Level Systems in the 2-Channel-Kondo Regime

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We point out a novel, non-universal contribution to the dephasing rate  $1/\tau_\varphi \equiv \gamma_\varphi$  of conduction electrons in metallic systems: scattering off non-magnetic two-level systems (TLSs) having almost degenerate Kondo ground states. In the regime  $\Delta_{\text{ren}} < T < T_K$  ( $\Delta_{\text{ren}}$  = renormalized level splitting,  $T_K$  = Kondo temperature), such TLSs exhibit non-Fermi-liquid physics that can cause  $\gamma_\varphi$ , which generally decreases with decreasing  $T$ , to seemingly saturate in a limited temperature range before vanishing for  $T \rightarrow 0$ . This could explain the saturation of dephasing recently observed in gold wires [Mohanty *et al.* Phys. Rev. Lett. **78**, 3366 (1997)].

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The dephasing behavior of conduction electrons in disordered systems in the zero-temperature limit has recently been subject to considerable and controversial discussions. The standard theory of dephasing in the context of weak localization [1], predicts that the dephasing rate  $1/\tau_\varphi \equiv \gamma_\varphi$  (extracted from the magnetoresistance) vanishes for  $T \rightarrow 0$ , since the phase space for inelastic scattering (e.g. electron-phonon or electron-electron) vanishes as the electron energy approaches the Fermi energy. In recent experiments on pure gold wires, however, Mohanty, Jariwala and Webb (MJW) [2] found that  $\gamma_\varphi$  saturated at a *finite* value for  $T \lesssim 1\text{K}$ , though two common “extrinsic” sources of dephasing, namely magnetic impurities and heating, were demonstrably absent. Pointing out a similar saturation in older data on various other 1D and 2D diffusive systems, MJW suggested [2] that the saturation could be due to a universal mechanism intrinsic to the sample, namely “zero-point fluctuations of phase coherent electrons”. Although this suggestion contradicts the standard view, Golubev and Zaikin [3] developed it into a detailed theory that was claimed to agree with numerous experiments. However, their theory was criticized, most strongly in [4], but also in [5,6]. In [4] it was suggested that MJW’s elaborate shielding precautions were insufficient and that external microwave fields caused the saturation.

In this Letter, we reexamine another source of dephasing, non-universal but intrinsic to any metal sample with structural disorder (which is never completely absent), namely *dynamical two-level systems* (TLSs), such as point defects associated with dislocations, interfaces, surfaces or amorphous regions. TLSs were not considered as source of dephasing in the above-mentioned debate (except very recently in [7]), since standard inelastic scattering off non-degenerate TLSs (assuming the standard uniform distribution of level splittings, as discussed below) gives  $\gamma_\varphi \sim T$  [8,9], which vanishes at low  $T$ .

Here, however, we point out that another dephasing

mechanism exists for TLSs in metals: these are known to act as non-magnetic or orbital 2-channel Kondo (2CK) impurities that exhibit non-Fermi-liquid (NFL) behavior in the regime  $\Delta_{\text{ren}} < T < T_K$  ( $\Delta_{\text{ren}}$  = renormalized level splitting,  $T_K$  = Kondo temperature), and we argue below that *this NFL behavior includes dephasing*; in fact, it can cause an apparent saturation in the decrease of  $\gamma_\varphi$  with decreasing  $T$  (although  $\gamma_\varphi$  does tend to zero for  $T \rightarrow 0$ ). This novel dephasing mechanism is *non-universal*, since the distribution of the material parameter  $T_K$  sets the energy scale, and since the density of TLSs depends on the history of the sample. Reasonable assumptions for the density of TLSs in Au lead to estimates for  $\gamma_\varphi$  in accord with the saturation behavior seen by MJW.

We start by noting that any dynamical impurity, i.e. one with internal degrees of freedom, can potentially dephase a conduction electron scattering off it: if in the process the impurity changes its state, the electron’s “environment changes”, and this, quite generally, causes dephasing [10]. (In contrast, static impurities cannot change their state and hence cannot cause dephasing).

In this Letter, we focus on dynamical “spin 1/2” impurities with two states, denoted by  $\uparrow$  and  $\downarrow$ , which scatter free conduction electrons according to the rather general interaction (specific examples are discussed below):

$$H_I = \sum_{\varepsilon \varepsilon'} \sum_{\alpha \alpha' j \mu} c_{\varepsilon \alpha j}^\dagger v_{\alpha \alpha'}^\mu c_{\varepsilon' \alpha' j} S_\mu. \quad (1)$$

The electrons are labeled by an energy  $\varepsilon$ , a “spin” index  $\alpha$  that is not necessarily conserved and a “channel” index  $j$  that (by definition) is conserved; the  $S_\mu$  ( $\mu = x, y, z$ ) are spin-1/2 operators, with  $S_z$  eigenvalues ( $\uparrow, \downarrow$ ) =  $(\frac{1}{2}, -\frac{1}{2})$ ; the coupling  $v^z$  describes the difference in scattering potentials seen by electrons scattering from the  $\uparrow$  or  $\downarrow$  state without flipping it, and is often called a “screening” interaction, since it generates a ( $S_z$ -dependent) screening cloud around the impurity; and  $v^x, v^y$  describe scattering processes that “flip the spin” of the impurity.

*Magnetic Impurities:*— As an illustrative example, let us briefly review dephasing for the 1-channel Kondo model, for which the channel index  $j = 1$  may be dropped and  $v_{\alpha\alpha'}^\mu = v\sigma_{\alpha\alpha'}^\mu$ . Let  $\gamma(T)$  be the scattering rate of an electron at the Fermi surface ( $\varepsilon = 0$ ); it can be split up as  $\gamma = \gamma_\varphi + \gamma_{\text{pot}}$  into parts that do or do not cause dephasing, respectively (“pot” for “potential” scattering). Two kinds of processes contribute to  $\gamma_\varphi$ : (i) spin-flip scattering, as explained above, and (ii) single-to-many particle scattering (see inset to Fig. 1), since additional electron-hole pairs can carry off phase information. Figure 1(a) shows the generic temperature-dependence of  $\gamma$ ,  $\gamma_{\text{pot}}$  and  $\gamma_\varphi$  [11]: As  $T$  approaches  $T_K$  from above, all three rates increase logarithmically. As  $T$  is decreased past  $T_K$ ,  $\gamma$  continues to increase monotonically, but crosses over to a  $(1 - \text{const} \times T^2)$  behavior; in contrast,  $\gamma_\varphi$  decreases (this has been observed directly in the magnetoresistance of samples containing magnetic impurities [2,12]), since below  $T_K$  the formation of a Kondo singlet between the impurity and its screening cloud begins to suppress spin-flip scattering. For  $T \ll T_K$  the singlet is inert (with spin-flip rate  $\sim e^{-T/T_K}$ ), and other conduction electrons experience only potential scattering off it; they hence form a Fermi-liquid, in which a weak residual interaction between electrons of opposite spins [Eq. (D5) of [13]] yields a dephasing rate  $\gamma_\varphi \propto T^2/T_K^2$ , which vanishes as  $T \rightarrow 0$ .

*TLSs in metals:*— Next we consider an atom or group of atoms moving in a double-well potential. Labeling the separate ground states of the “left” and “right” well by  $(L, R) \equiv (\uparrow, \downarrow)$ , the bare Hamiltonian  $\Delta_z S_z + \Delta_x S_x$  describes a TLS with energy  $\Delta_z$ , spontaneous transition rate  $\Delta_x$  and level splitting  $\Delta = \sqrt{\Delta_z^2 + \Delta_x^2}$  between the ground and excited states, say  $|\pm\rangle$ . It is common [9] to assume a constant distribution  $P(\Delta) = \bar{P}$  of TLSs, with  $\bar{P} \simeq 10^{19} - 10^{20} \text{ eV}^{-1} \text{ cm}^{-3}$  in metallic glasses.

When put in a metal, such a TLS will scatter conduction electrons. The interaction’s most general form is given by Eq. (1), where now the “spin” index  $\alpha$  classifies the electron’s orbital state, representing e.g. its angular momentum  $(l, m)$ , and the “channel” index  $j = (\uparrow, \downarrow)$  denotes its Pauli spin, which is conserved since the TLS is non-magnetic. This is in effect a generalized 2-channel Kondo interaction, with which one can associate a Kondo temperature  $T_K$ . In general it is highly anisotropic, with  $|v^x|, |v^y| \ll |v^z|$ , since  $v^x, v^y$  describe electron-assisted inter-well transitions and depend on the barrier size much more strongly than the screening interaction  $v^z$  does.

*Slow fluctuators:*— If the barrier is sufficiently large ( $|v^x|, |v^y| \ll |v^z|$ , so that  $T_K \ll T, \Delta_x, \Delta_z$  and Kondo physics is not important), the system is a “slow fluctuator”, which can adequately be described by the so-called “commutative” model, in which one sets  $v^x = v^y = 0$  from the outset [9,14]. This model does not renormalize to strong coupling at low temperatures, and  $\Delta$  is renormalized downward only slightly (by at most a few %) [15]. To estimate  $\gamma_\varphi$ , one may thus use the bare parameters

and perturbation theory in  $v^z$ , which couples  $[9] |+\rangle$  and  $|-\rangle$ . Since  $v^z$ -scattering between these, being inelastic, requires  $T > \Delta$ , the  $\Delta$ -averaged inelastic scattering rate is  $\bar{\gamma}_{\text{inel}} \propto T$  (provided that  $(\Delta_x)_{\text{max}}, (\Delta_z)_{\text{max}} > T$ , [8,9]). Thus  $\bar{\gamma}_\varphi \propto T$  too, which does not saturate as  $T \rightarrow 0$ .

*Fast TLSs:*— For sufficiently small inter-well barriers, however, the effective  $T_K$  of a TLS can be significantly larger than its effective level splitting, so that Kondo physics does come into play [16]. Such TLSs require the use of the full “non-commutative” model with  $v^x$  and  $v^y \neq 0$ , which flows toward strong coupling under the renormalization group (RG) [17,18]. Extensive RG studies [19,20] showed that the regime  $T \lesssim T_K$  is governed by an effective isotropic 2CK interaction of the form (1) with  $\alpha = (1, 2)$  (since all but the two most-strongly-coupled orbital states decouple) and  $v_{\alpha\alpha'}^\mu = v\sigma_{\alpha\alpha'}^\mu$ , and with an effective renormalized splitting  $\Delta_{\text{ren}} = \Delta^2/T_K$ . In the so-called *NFL regime*  $\Delta_{\text{ren}} < T < T_K$ , the resulting effective 2CK model exhibits NFL behavior [13,21]. The zero-bias anomalies observed in recent years in nanoconstrictions made from a number of different materials, such as Cu [22], Ti [23] or metallic glasses [24,25], can be consistently explained by attributing them to fast TLSs in or near this 2CK NFL regime [26,27]. The Kondo temperatures of the relevant TLSs were deduced in [22–24] from the width of the zero-bias anomalies to be  $T_K \gtrsim 1\text{K}$ , and in [25] the insensitivity of the anomalies to a high-frequency modulation of the bias voltage implied  $T_K \gtrsim 2\text{K}$ .

*2CK Dephasing:*— Let us now consider dephasing due to fast TLS in the NFL regime, a matter that to our knowledge has not been addressed before. In the NFL regime the single-to-single- and single-to-many-particle scattering rates  $\gamma_{\text{ss}}(T)$  and  $\gamma_{\text{sm}}(T)$  (inset of Fig. 1) are known to respectively decrease and increase with decreasing  $T$ , in such a way that the full scattering matrix is unitary [28]. Now, our key point is that *single-to-many-particle scattering must cause dephasing*, so that we can take  $\gamma_\varphi \simeq \gamma_{\text{sm}}$ . This immediately implies that the dephasing rate *increases with decreasing temperature* in the NFL regime, as indicated schematically in Fig. 1(b). In fact, for  $\Delta_{\text{ren}} = 0$ , one actually has  $\gamma_{\text{ss}} \propto (T/T_K)^{1/2} \rightarrow 0$  as  $T \rightarrow 0$  [28], implying that the dephasing rate ( $= \gamma_{\text{sm}}$ ) would be finite even at  $T = 0$ . To heuristically understand this result, recall that the NFL fixed point describes an overscreened impurity that has a non-zero ground state entropy of  $\frac{1}{2} \ln 2$  [21] and cannot be viewed as an inert object (in contrast to 1CK case, where the ground state singlet has entropy 0); intuitively speaking, it is the dynamics associated with this residual entropy that causes dephasing even at  $T = 0$ .

Generally, however,  $\Delta_{\text{ren}} \neq 0$ ; for  $T < \Delta_{\text{ren}} = \Delta^2/T_K$ , FL behavior is restored [20] and  $\gamma_\varphi$  drops back to zero, so that we crudely take  $\gamma_\varphi(T) \simeq \gamma_{\text{sm}}(T) \theta(\sqrt{TT_K} - \Delta)$ . Since NFL physics also requires  $\Delta < T_K$ , we estimate the  $\Delta$ -averaged dephasing rate (with  $P(\Delta) = \bar{P}$ ) as

$$\bar{\gamma}_{\varphi}^{T_K} \simeq \int_0^{T_K} d\Delta P(\Delta) \gamma_{\varphi}(T), \quad (2)$$

which yields  $\bar{\gamma}_{\varphi}^{T_K}(T) \simeq \bar{P} \gamma_{\text{sm}}(T) \min[\sqrt{TT_K}, T_K]$ . This has a broad peak around  $T_K$  [Fig. 1(c), dotted line]. To next average over  $T_K$ , we assume that the distribution  $P(T_K)$  has a broad maximum near, say,  $\bar{T}_K$ . Then the peak of  $\bar{\gamma}_{\varphi}^{T_K}(T)$  would be broadened for  $\bar{\gamma}_{\varphi}(T) = \int dT_K P(T_K) \bar{\gamma}_{\varphi}^{T_K}(T)$  into a flattened region near  $\bar{T}_K$ . Adding to this a power-law decay due to other sources of dephasing, e.g.  $\gamma_{\varphi}^{\text{1D}} \propto T^{2/3}$ , the usual result for disordered 1D wires [1], the total dephasing rate  $\gamma_{\varphi}^{\text{tot}} = \bar{\gamma}_{\varphi} + \gamma_{\varphi}^{\text{1D}}$  would have a broad shoulder around  $\bar{T}_K$ , while vanishing for  $T \rightarrow 0$  [Fig. 1(c), solid line]. Thus *2CK impurities can cause the total dephasing rate  $\gamma_{\varphi}^{\text{tot}}(T)$  to seemingly saturate in a limited temperature range.*

*Estimate of numbers:*— The shape of  $\gamma_{\varphi}^{\text{tot}}(T)$  and the existence of the broad shoulder depend on  $P(T_K)$ ,  $\bar{T}_K$  and the relative weights of  $\bar{\gamma}_{\varphi}$  and  $\gamma_{\varphi}^{\text{1D}}$ . To predict these from first principles would be overly ambitious, since a microscopically reliable model for the TLSs and their couplings to electrons is not available. Instead, let us use MJW’s data to infer what properties would be needed to attribute their saturation to 2CK dephasing, and check the inferred properties against other studies of TLSs.

The dephasing times in Au wires saturated at  $\tau_{\varphi} \simeq 5$  to 0.5ns below a crossover temperature of about  $T^* \simeq 1\text{K}$ , which we associate with  $\bar{T}_K$ . We further assume the saturation to be dominated by TLSs with  $\Delta_{\text{ren}} < T^* < T_K$ , i.e. with  $\Delta < 1\text{K} < T_K$ . Such parameters are reasonable, since experiment [22–25] and theory [16] suggest that a sizable fraction of  $\Delta < 1\text{K}$  TLSs indeed do also have  $T_K > 1$ . Let us estimate their required density. Impurities with dephasing cross-section  $\sigma_{\varphi}$  and density  $n_i$  yield a dephasing rate  $\gamma_{\varphi} = v_F n_i \sigma_{\varphi}$ . The density of strongly-coupled fast TLSs, i.e. with  $\sigma_{\varphi} \lesssim \sigma_{\text{unit}}$  close to the unitarity limit  $\sigma_{\text{unit}} = 4\pi/k_F^2$  per electron species, would thus have to be of order  $n_i = 1/(\tau_{\varphi} v_F \sigma_{\text{unit}}) \gtrsim 2 \times (10^{15} - 10^{16})\text{cm}^{-3}$  (which is rather small: given the atomic density in Au of  $6 \times 10^{22}\text{cm}^{-3}$ ,  $n_i$  implies a TLS density of only 0.02 – 0.2 ppm [29]).

The estimated value for  $n_i$  is reasonable too: in metallic glasses, the density of TLSs with splittings  $\Delta < 1\text{K}$  is  $\bar{P} \times 1\text{K} \simeq 9 \times (10^{14} - 10^{15})\text{cm}^{-3}$ ; in polycrystalline Au, which is often taken to have roughly the same density of TLSs as metallic glasses [30], it is probably somewhat larger, since (i) in polycrystals, which constitute a more symmetric environment than glasses, the TLS distribution is probably more heavily weighted for small splittings; (ii) in 1D wires, surface defects can increase the total density of TLSs, and (iii) the bare splittings  $\Delta_z, \Delta_x$  are renormalized downward during the flow toward the NFL regime [20]. The density of TLS in Au wires that can be expected to cause 2CK dephasing thus compares satisfactorily with  $n_i$  estimated above.

*Possible Checks:*— We emphasize that the 2CK dephasing mechanism is non-universal: firstly, the energy scale is set by  $T_K$ , and secondly, whether a sample contains sufficiently many TLSs to cause appreciable dephasing depends on its history. Thus, if the TLSs can be modified or even removed, e.g. by thermal cycling or annealing [22], the dephasing behavior should change significantly or even disappear. Drawn wires containing more dislocations (which may act as TLSs) should show stronger 2CK dephasing than evaporated wires [31]. Actually, already in 1987 Lin and Giordano [32] found hints in Au-Pd films of a low-temperature dephasing mechanism that is “very sensitive to metallurgical properties”. In semiconductors, however, TLSs are unlikely to exhibit 2CK dephasing, since the much smaller electron density implies much smaller couplings (for recent dephasing experiments on semiconductors, see [4]).

In summary, we have pointed out a new, non-universal mechanism by which two-level systems in metals, acting as 2CK impurities, can cause dephasing, namely through an increased single-to-many-particle scattering rate in their non-Fermi-liquid regime. We estimate that the Au wires of MJW [2] contain sufficiently many TLSs to yield 2CK dephasing rates comparable to the saturation rates observed there. More generally, though, the 2CK dephasing mechanism could be used to diagnose 2CK non-Fermi-liquid behavior in other metals containing TLSs.

*Note added:*— Concurrent with this work, Imry, Fukuyama and Schwab [7] proposed that  $1/f$  noise from TLSs might produce essentially  $T$ -independent dephasing by a different mechanism (not involving any 2CK physics), if  $(\Delta_x)_{\text{max}}$  is assumed to be  $\ll T$  even for  $T \simeq 1\text{K}$ , rather than the more common assumption [8,9] that  $\Delta_x$  has a larger range.

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and qualitatively [Ralph *et al.* Phys. Rev. Lett. **75**, 771 (1995); **75**, 2786(E), (1995)] (see [26] for a detailed discussion). WAM's criticism of the 2CK scenario is countered at length by G. Zaránd and A. Zawadowski [Physica (Amsterdam), **218B**, 60 (1996)], and in [18,34].

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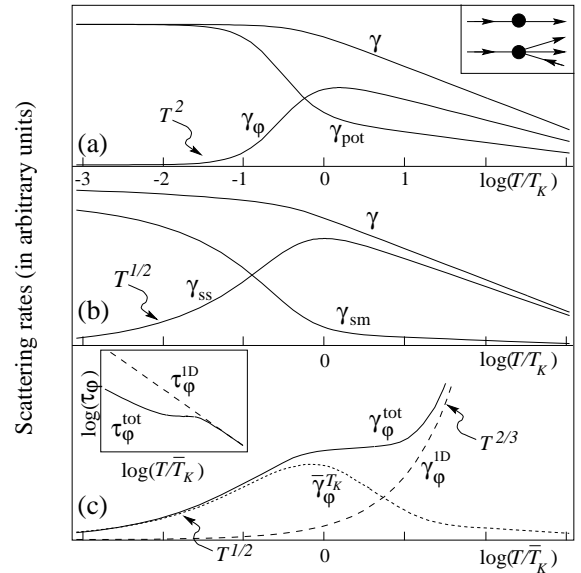


FIG. 1. Sketch of scattering rates as functions of  $\log(T/T_K)$  for (a) the isotropic 1CK and (b) the anisotropic 2CK models (for  $\Delta_{\text{ren}} = 0$ ); inset: single-to-single- and single-to-many-particle scattering. (c) Dotted line: a  $\Delta$ -averaged 2CK dephasing rate  $\bar{\gamma}_\phi^{TK}$  with  $T_K \simeq \bar{T}_K$  (averaging such curves over  $T_K$  yields  $\bar{\gamma}_\phi$ ); dashed line:  $\gamma_\phi^{1D} \sim T^{2/3}$ ; full line:  $\gamma_\phi^{\text{tot}} = \bar{\gamma}_\phi + \gamma_\phi^{1D}$ ; inset: the corresponding dephasing times.